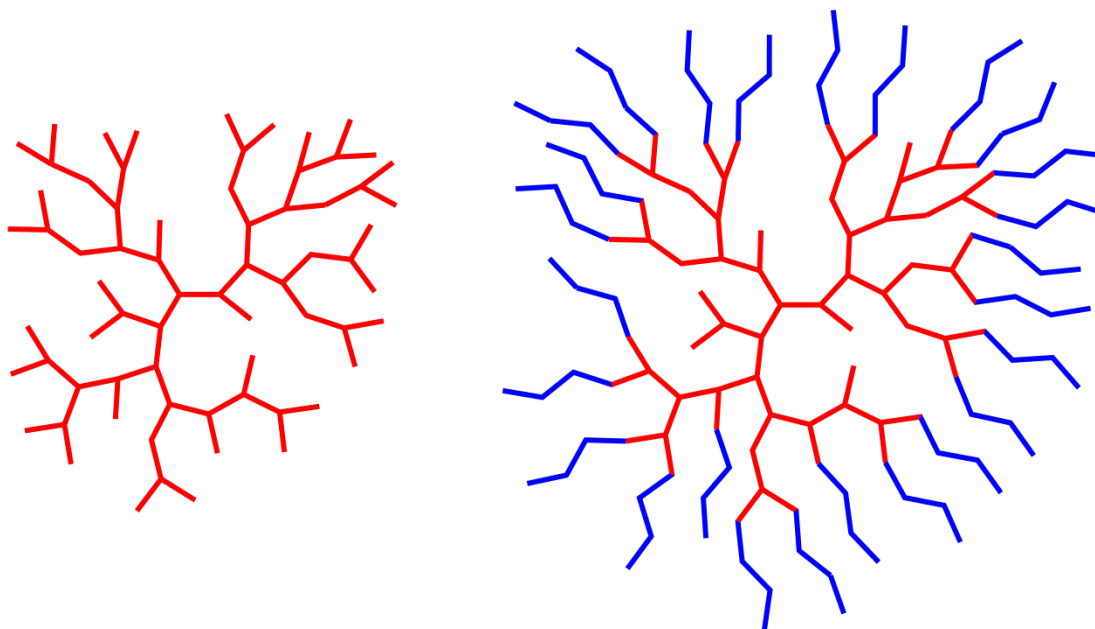


# ***HBP Builder*: A Tool to Generate Hyperbranched Polymers and Hyperbranched Multi-Arm Copolymers for Coarse-grained and Fully Atomistic Molecular Simulations**

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**Figure S1.** Schematic representation of HBPs and HBMCs. Red blocks are hydrophobic hyperbranched core while blue ones are hydrophilic linear arms.

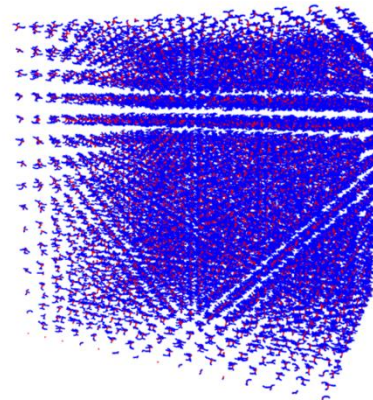
(a)

Figure S2(a) shows the input dialogue box for HBP Builder\_CG. The box contains various parameters for generating HBMCs structures, including:

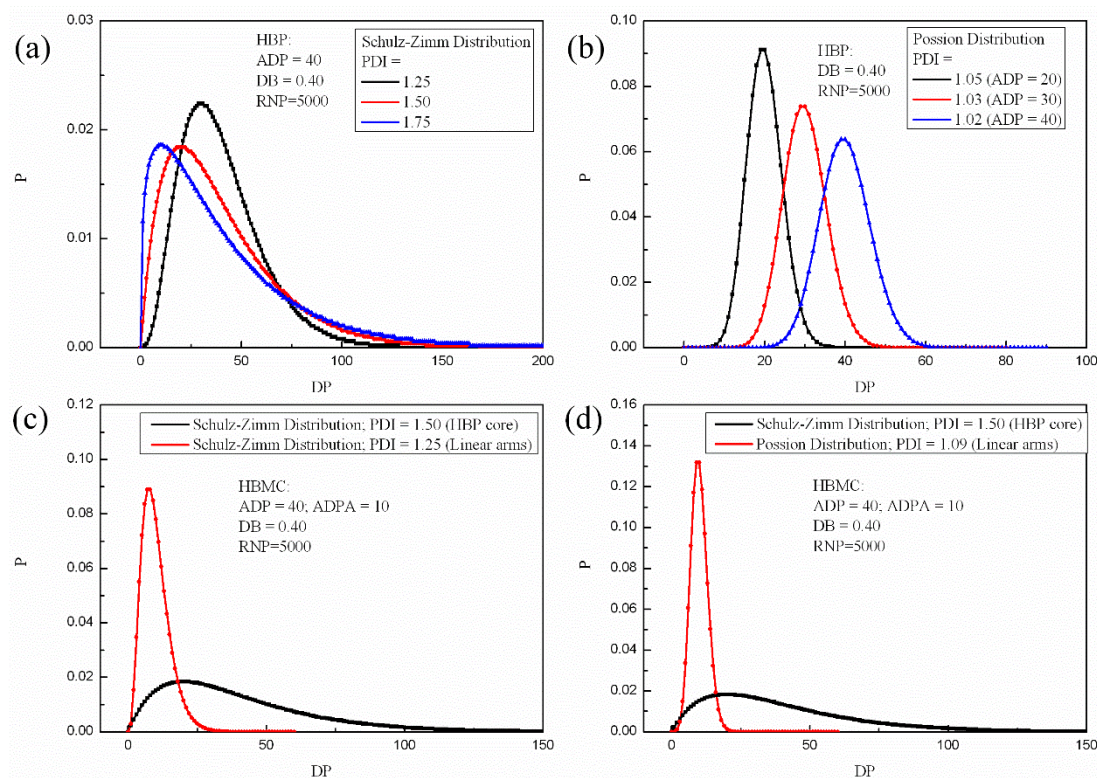
- Average degree of polymerization of the hyperbranched core ( $\geq 3$ ): 60
- Required number of the HBMCs ( $\geq 1$ ): 3000
- Polydisperse distribution model of the hyperbranched core (Poisson(1) or Schulz-Zimm(0)): 0
- Polydispersity index of the hyperbranched core ( $\geq 1$ ): 1.5
- Branch number of the root node ( $\geq 2$ ): 3
- Degree of branching of the hyperbranched core (0-1): 0.4
- Branch number of the terminal unit (0,1,2): 2
- Graft ratio of the arm unit (0-1): 0.5
- Average degree of polymerization of the arm unit ( $\geq 0$ ): 5
- Polydisperse distribution model of the arm unit (Poisson(1) or Schulz-Zimm(0)): 0
- Polydispersity index of the arm unit ( $\geq 1$ ): 1.16

Buttons: Save, Run, Quit

(b)



**Figure S2.** Simulation box with various HBMCs structures generated by HBP Builder\_CG. The input dialogue (a); The generated simulation box with polydisperse HBMCs (b).



**Figure S3.** Schulz-Zimm distributions of HBPs (a); Poisson distributions of HBPs (b); Schulz-Zimm distributions of HBMCs (c); Schulz-Zimm/Poisson distributions of HBMCs. In each figure, the solid lines represent the calibration curves and the points represent the distribution generated by HBP Builder. ADP represents the average degree of polymerization of HBP; ADPA represents the average degree of polymerization of linear arms; RNP represents the required number of the polymers; DP represents the degree of polymerization; P represents the normalized distribution probability. As shown in Figures S3a and S3b, all the HBPs generated by HBP Builder (data points) totally conform to the theoretical predications from Schulz-Zimm or Poisson distribution (continuous lines). Meanwhile, both the arms and the HBP cores of HBMCs generated by HBP builder also conform to the theoretical predications from Schulz-Zimm or Poisson distribution very well (Figures S3c and S3d).

**Table S1.** The map file of HPG-star-PEG.

Type	File location	Joint point number	Atom index
A3_0	mol2//a30.mol2	3	19 21 23
A3_1	mol2//a3.mol2	3	13 10 12
A2_1	mol2//a2.mol2	2	13 10
A2_2	mol2//a2.mol2	2	13 12
A1_1	mol2//a2.mol2	1	13
A11_1	mol2//a2.mol2	2	13 10
A11_2	mol2//a2.mol2	2	13 12
A12	mol2//a2.mol2	3	13 10 12
L1	mol2//peg.mol2	1	3

**Table S2.** The Running time(t) of several studied systems.

RNP	DP	PDI_core PDI_arm	BRT	DB	GRA	DP_arm	t (s)
10	22	1.0/1.0	3	0.4	1.0	5	<1
10	46	1.0/1.0	3	0.5	1.0	5	<1
100	66	1.0/1.0	3	0.6	1.0	5	1
1000	40	1.0/1.0	3	0.4	1.0	10	27
1000	40	1.5/1.2	3	0.4	1.0	10	26
1000	40	1.5/1.2	4	0.4	1.0	10	27
1000	60	1.5/1.2	3	0.4	1.0	10	52
1000	60	1.5/1.2	4	0.4	1.0	10	50
1000	80	1.5/1.2	3	0.4	1.0	10	88
1000	80	1.5/1.2	4	0.4	1.0	10	84
2000	80	1.5/1.2	3	0.4	1.0	20	421
3000	80	1.5/1.2	3	0.4	1.0	20	900